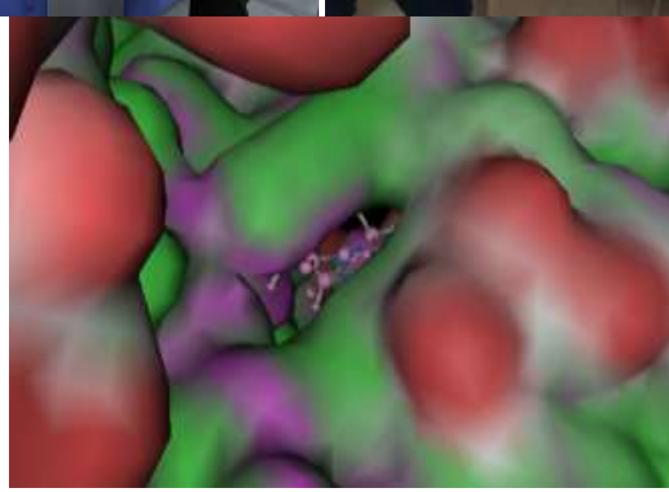
SHIV NADAR UNIVERSITY

Department of Chemistry

School of Natural Sciences

Course Catalogue & Program Structure 2018



Department of Chemistry

Chemistry forms the link between the fundamental principles governing the nature of the universe and the science of life. Chemistry education at SNU provides focus on a variety of inter-disciplinary areas, spanning different scientific disciplines as well as non-traditional areas in the arts and humanities, *e.g.* a Major in Chemistry can be combined with a Minor in Bioinformatics at SNU. Or you can pursue a Major in Chemistry with a specialization in either Chemical Physics or Chemical Biology.

Our research programs reach across the campus and beyond, linking together departments, schools, inter-disciplinary centers and internship opportunities in the chemical industry and national labs. University-wide elective courses in the curriculum allow students unprecedented freedom to explore subjects outside their chosen major, in some depth. This flexible and broad curriculum prepares students not just for a career in chemistry upon graduation, but for a leadership role in the world as well.

The Undergraduate Chemistry Experience

The chemistry curriculum at SNU provides both a broad background in chemical principles and in-depth study of chemistry or chemistry-related areas that build on this background. The chemistry curriculum is divided into three categories: introductory general chemistry, foundation courses providing breadth across sub-disciplines, and rigorous in-depth courses that build upon these foundations and develop critical thinking and problem-solving skills. Since chemistry is an experimental science, substantial laboratory work is an integral part of almost all our courses. The introductory general chemistry course provides a common grounding in basic chemical concepts for students with diverse backgrounds, develops basic mathematical and laboratory skills, and prepares students for the foundation courses. Foundation courses in analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry provide breadth and lay the groundwork for more in-depth course work.

Laboratory Experience: The chemistry laboratory experience at SNU includes synthesis of molecules; measurement of chemical properties, structures, and phenomena; hands-on experience with modern analytical instrumentation; and computational data analysis and modelling. All laboratory programs are conducted in a safe environment that includes adherence to national and state regulations regarding hazardous waste management and laboratory safety including, facilities for chemical waste disposal, safety information and reference materials, and personal protective equipment available to all students and faculty. The chemistry laboratories at SNU are equipped with functioning fume hoods, safety showers, eyewashes, first aid kits, and fire extinguishers must be readily available. Students are trained in modern chemical safety, to understand responsible disposal techniques, understand and comply with safety regulations, understand and use material safety data sheets (MSDS), recognize and minimize potential chemical and physical hazards in the laboratory, and know how to handle laboratory emergencies effectively.

Problem-Solving Skills: As part of the SNU experience, students will be expected to develop the ability to define problems, develop testable hypotheses, design and execute experiments, analyze data using statistical methods, and draw appropriate conclusions. The chemistry curriculum provides ample opportunities for developing both written and oral communication skills, as well as team skills. Our instructional programs incorporate team experiences in classroom and laboratory components of the chemistry curriculum.

Careers in Chemistry Chemistry forms the scientific basis for a wide variety of career options, ranging from traditional areas such as academics, pharmaceuticals, chemical analysis and synthesis, quality control and quality assurance, to inter-disciplinary fields such as molecular biology, materials science and biophysics, and non-traditional areas such as medicine, patent or environmental law, forensic science, technical writing, art conservation, environmental studies, *etc*.

Undergraduate Research in Chemistry

Research activities are not confined to post-graduate level, but are integrated into the under-graduate program at SNU through our REAL (Research Experiential & Applied Learning) courses. Undergraduate research allows students to integrate and reinforce chemistry knowledge from their formal course work, develop their scientific and professional skills, and create new scientific knowledge. Original research culminating in a comprehensive written report provides an effective means for integrating undergraduate learning experiences, and allows students to participate directly in the process of science. Opportunities for research in chemistry at SNU are available in the following broad areas:

- Catalysis
- Chemical Biology
- Cheminformatics
- Chemistry of Nanomaterials
- Computational Quantum Chemistry
- Coordination Chemistry
- Green Chemistry
- Medicinal Chemistry
- Molecular Toxicology
- Polymer Chemistry
- Structural Chemistry and Crystallography
- Supramolecular Chemistry
- Synthetic Organic Chemistry

Major in Chemistry

The basic undergraduate degree program offered by the Department of Chemistry is the Bachelor of Science: B.Sc. (Research) in Chemistry.

Every chemistry undergraduate student of the University is required to take a number of credits from courses broken up into the following categories:

a) CCC (Common Core Curriculum courses offered by the university)
b) UWE (University Wide Electives; courses so designated and offered by departments other than Chemistry)
c) Introductory Chemistry courses (CHY100 – 199)
d) Foundation Chemistry courses (CHY200 – 299)
e) In-Depth Chemistry courses (CHY300 – 499)
f) Advanced Electives (CHY400 – 599)

The credit requirements for **B.Sc (Research) Chemistry** are:

116 credits = 70 credits in compulsory Chemistry courses (12 Introductory + 29 Foundation + 29 In-Depth) + 28 required Physics/Maths/Life Sci/CS + 6 credits Chemistry electives + 12 credits Senior Project.

+ 42 UWE/CCC credits with a minimum of 18 from each.

Minor in Chemistry

Undergraduate students of the university who are not majoring in Chemistry have the option to take a Minor in Chemistry. **Academic Requirements for Chemistry Minor: 24** credits = 10 credits in Introductory courses + 11 credits in Foundation courses:

CHY111	Chemical Principles	5 credits
CHY122	Basic Organic Chemistry I	4 credits
CHY142	Main Group Chemistry	3 credits
CHY211	Chemical Equilibrium	5 credits
CHY213	Physical Methods in Chemistry	4 credits

+ 3 credits chosen from the Chemistry In-Depth/Elective courses.

Chemistry Course Catalogue

The chemistry program at SNU provides both a broad background in chemical principles and in-depth study of chemistry or chemistry-related areas that build on this background. The chemistry curriculum is divided into three parts: (1) the introductory chemistry experience, (2) foundation course work that provides breadth, and (3) rigorous in-depth course work that builds on the foundation. Because chemistry is an experimental science, substantial laboratory work is an integral part of this experience.

Introductory or General Chemistry: The introductory or general chemistry experience plays a vital role in educating all students. The introductory courses provide a common background for students with a wide range of high school experiences, and allow a period for consolidation of chemical concepts, as well as mathematical and laboratory skills. For students pursuing a chemistry major, the introductory chemistry courses provide preparation for the foundation course work, ensuring that students know basic chemical concepts such as stoichiometry, states of matter, atomic structure, molecular structure and bonding, thermodynamics, equilibria, and kinetics. Students also need to be competent in basic laboratory skills such as safe practices, keeping a notebook, use of electronic balances and volumetric glassware, preparation of solutions, chemical measurements using pH.

CHY111: **Chemical Principles** (5 credits: 4 Lectures/Tutorial + 3-hour Lab) Monsoon

This course will focus on introductory chemical principles, including periodicity, chemical bonding, molecular structure, equilibrium and the relationship between structure and properties. Students will explore stoichiometric relationships in solution and gas systems which are the basis for quantifying the results of chemical reactions. Understanding chemical reactivity leads directly into discussion of equilibrium and thermodynamics, two of the most important ideas in chemistry. Equilibrium, especially acid/base applications, explores the extent of reactions while thermodynamics helps us understand if a reaction will happen. The aim of the laboratory will be to develop your experimental skills, especially your ability to perform meaningful experiments, analyze data, and interpret observations. This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

COURSE CONTENT:

1. Atomic structure, Periodic table, VSEPR, Molecular Orbital theory, and biochemistry**:**

    a. Introduction: why chemistry in engineering? Concept of atom, molecules, Rutherford's atomic model, Bohr's model of an atom, wave model, classical and quantum mechanics, wave particle duality of electrons, Heisenberg's uncertainty principle, Quantum-Mechanical Model of Atom, Double Slit Experiment for Electrons, The Bohr Theory of the Hydrogen atoms, de Broglie wavelength, Periodic Table.

b. Schrodinger equation (origin of quantization), Concept of Atomic Orbitals, representation of electrons move in three-dimensional space, wave function (Ψ), Radial and angular part of wave function, radial and angular nodes, Shape of orbitals, the principal (n), angular (l), and magnetic (m) quantum numbers, Pauli exclusion principle.

c. Orbital Angular Momentum (l), Spin Angular Momentum (s), spin-orbit coupling, HUND's Rule, The *aufbau* principle, Penetration, Shielding Effect, Effective Nuclear Charge, Slater's rule.

d. Periodic properties, Ionization Energies of Elements, Electron affinities of elements, Periodic Variation of Physical Properties such as metallic character of the elements, melting point of an atom, ionic and covalent nature of a molecule, reactivity of hydrides, oxides and halides of the elements.

e. Lewis structures, Valence shell electron pair repulsion (VSEPR), Valence-Bond theory (VB), Orbital Overlap, Hybridization, Molecular Orbital Theory (MO) of homo-nuclear and hetero-nuclear diatomic molecules, bonding and anti-bonding orbitals.

f. Biochemistry: Importance of metals in biological systems, Fe in biological systems, Hemoglobin, Iron Storage protein - Ferritin]

2. Introduction to various analytical techniques:

Introduction to Symmetry operations

UV-Visible Spectroscopy, IR Spectroscopy, NMR spectroscopy, X-Ray crystallography

Spectroscopy: Regions of Electromagnetic Radiation, Infra-Red (IR) Spectroscopy or Vibrational Spectroscopy of Harmonic oscillators, degree of freedom, Stretching and Bending, Infrared Spectra of different functional groups such as OH, NH_2, CO_2H etc., UV-Vis Spectroscopy of organic molecules, Electronic Transitions, Beer-Lambert Law, Chromophores, principles of NMR spectroscopy, ^1H and ^{13}C-NMR, chemical shift, integration, multiplicity,

X-ray crystallography: X-ray diffraction, Bragg's Law, Crystal systems and Bravais Lattices

3. **The Principles of Chemical Equilibrium, kinetics and intermolecular forces:**
   - Heat & Work; State Functions
   - Laws of thermodynamics
   - Probability and Entropy

- Thermodynamic and Kinetic Stability
- Determination of rate, order and rate laws
- Free Energy, Chemical Potential, Electronegativity
- Phase Rule/Equilibrium
- Activation Energy; Arrhenius equation
- Catalysis: types; kinetics and mechanisms
- Electrochemistry
- Inter-molecular forces

4. Introduction to organic chemistry, functional group and physical properties of organic compounds, substitution and elimination reaction, name reactions and stereochemistry

Prerequisite: None.

CHY120: **Molecules and Medicines** (3 credits: 3 Lectures) Spring [UWE]

Since the time of Hippocrates until modern days, human being has explored several means of alleviating pain and curing disease. There have been pathbreaking discoveries resulting in the development of medicines of immense benefit. Present day research of inventing novel molecules constantly adds to the repertoire of drugs available to counter ill-health.

We will begin with a short introduction (which discusses fundamental organic chemistry followed by development and testing of drugs). Next we will explore the discovery and development of a range of drugs and medicines that relieve pain, effect cures and reduce the symptoms of ill-health. We will discuss how drugs interact with and affect their target areas in the human body. There are online videos to help you to understand the three-dimensional structures and shapes of the molecules concerned and to develop an understanding of how the drugs work.

Prerequisite: None.

CHY122: **Basic Organic Chemistry-I** (4 credits: 2 Lectures+ 1 Tutorial + 3-hour Lab) Spring

This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

COURSE CONTENT:

1. Intermolecular forces of attraction: van der Waals forces, ion-dipole, dipole-dipole and hydrogen bonding
2. Homolytic and heterolytic bond fission.
3. Hybridization- Bonding
4. Electron displacements: Inductive, electromeric, resonance, hyperconjugation effect
5. Reaction intermediate- their shape and stability
    a. carbocations,
    b. carbanions,
    c. free radicals,
    d. carbenes,
    e. benzynes

6. Acidity and basicity of organic molecules: Alkanes/Alkenes, Alcohols/Phenols/Carboxylic acids, Amines pKa, pKb.
7. Electrophiles and nucleophiles. Nucleophilicity and Basicity
8. Aromaticity and Tautomerism
9. Molecular chirality and Isomerism
    a. Cycloalkanes (C3 to C8): Relative stability, Baeyer strain theory and Sachse Mohr theory.
    b. Conformations and Conformational analysis: Ethane, n-butane, ethane derivatives, cyclohexane, monosubstituted and disubstituted cyclohexanes and their relative stabilities.
10. Stereochemistry (Structural- and Stereo-isomerism)
    a. Molecular representations: Newman, Sawhorse, Wedge & Dash, Fischer projections and their inter conversions.
11. Geometrical isomerism in unsaturated and cyclic systems: cis–trans and, syn-anti isomerism, E/Z notations. Geometrical isomerism in dienes- Isolated and conjugated systems, determination of configurations.
12. **Chirality and optical isomerism**: Configurational isomers. Molecules with one or two chiral centres- constitutionally symmetrical and unsymmetrical molecules; Enantiomers and diastereomers. Optical activity, disymmetry, meso compounds, racemic modifications and methods of their resolution; stereochemical nomenclature: erythro/threo, D/L and R/S nomenclature in acyclic systems. Measurement of optical activity: specific rotation.

Prerequisite: Chemical Principles (CHY111).

CHY140: **Chemistry of Colour and Art** (3 credits: 2 Lectures+ 2-hour Lab) Spring [REAL, UWE]

This inter-disciplinary course will introduce students to the basic principles of optics, colour theory and the chemical principles behind the colours of gemstones, pigments and nanomaterials. Absorption, scattering and emission of light, changes associated with chemical reactions, thermal radiation, colour vision, colours of bulk materials and at the nanoscale will be discussed and demonstrated. Topics covered include spectroscopy, art forensics, colour theory in art, colour spaces, colour in culture, introduction to photography, drawing and painting. Students will also explore how artists through the ages have used and exploited colour, and will have the opportunity to discover for themselves the fundamentals of colour photography, painting and art. **Lab and studio sessions will be conducted during alternate weeks**. Field trips to natural locations, art galleries and museums will be included to provide opportunities for creating individual works of art.

Prerequisite: None.

CHY142: **Main Group Chemistry** (3 credits: 2 Lectures+ 1 Tutorial) Spring

This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

COURSE CONTENT:

<u>The s–block elements and the noble gases:</u>

i) The s–block elements of Gr – I, Gr – II, their general electronic configuration, trends in I. P., ionic radii; reaction with H, O, N, C, and hydrolytic behaviour of the products.

ii) General metallurgical consideration of these elements.

iii) Differences of Li and Be from other members of their groups (the diagonal relationship).

iv) Isotopes of H, industrial preparation of deuterium, its properties, reactions and uses; ortho–para – hydrogen.

v) Separation and uses of the noble gases; compounds of Kr and Xe – preparation, properties, structures.

<u>The p–block elements:</u>

i) Gr. III. (a) The general group properties * (b) Boron Chemistry – preparation, properties of boranes; Structure and bonding of diborane, Boranine Boron nitrides; electron deficient nature of hydrides, halides and their polymerisation.

ii) Gr. IV (a) The general group properties * (b) Aspects of C and Si chemistry the difference of C and P from the rest of the group elements. Preparation, properties, u ses of the fluoroecarbons, the silanes and the silicones.

iii) Gr. IV (a) The general group properties * (b) N and P – Chemistry: The presence of lone pair and basicity of trivalent compounds; trends in bond angles of hydrides, halides, preparation, properties, structures and bonding of hydrazine, hydroxylamine, hydrazoic acids, the oxides and oxyacids of N, P; d – orbital participation in P–compounds.

iv) Gr. VI (a) The general group properties * (b) S–Chemistry – Preparation, properties, structures and bonding of the oxides, oxyacids (including the thionous, thionic and per–acids), halides, oxy–halides and poly sulphides; d–orbital participation in S–Compounds.

v) Gr. VII (a) The general group properties * (b) The halogen hydrides, their acidity; Preparation, properties, structures and bonding of the oxides and oxy acids; the inter halogen compounds including polyhalides, the pseudohalides – including their preparation, properties, structures. The cationic compounds of iodine.

* Note : General group properties : – For each group this includes discussion, on a comparative basis, of major physical and chemical properties, e.g. – i) Physical properties – the electronic configuration; ionisation potential / electron affinity; m.p. – b.p. ; ionic/covalent radii etc. ii) Chemical properties – Various oxidation states and their relative stability (redox behaviour in solution, wherever applicable), higher stability of the higher oxidation states for the heavier members; gradual changes of the ionic/covalent character of the compounds from lighter to heavier members; the relative acidity, amphoteric, basic characteristics of the oxides and formation of oxocations (wherever applicable); examples of compounds in all the oxidation states, in particular, the unusual (rare) oxidation states being stabilised through coordination; hydrides, halides (including the halo complexes) and their hydrolytic behaviour; dimerization and/or polymerization through halogen bridges (wherever applicable) etc. iii) Common natural sources of the elements.

Acid-Base / Ionic Equilibrium / Non-aqueous solvents, reduction.

Prerequisite: Chemical Principles (CHY111).

<u>Foundation Courses</u>: Foundation courses provides breadth and lays the groundwork for the in-depth course work in each of the five major areas of chemistry: analytical chemistry, biochemistry, inorganic chemistry, organic chemistry, and physical chemistry. The chemistry laboratory experience at SNU includes synthesis of molecules; measurement of chemical properties, structures, and phenomena. Students get hands-on experience with modern instrumentation on a variety of analytical instruments, including spectrometers, and are expected to understand the operation and theory of modern instruments and use them to solve chemical problems as part of their laboratory experience.

CHY211: **Chemical Equilibrium** (5 credits: 3 Lectures + 1 Tutorial + 3-hour Lab) Monsoon

In this course, we adopt a case studies approach to understanding thermodynamic principles already familiar to students from earlier courses. In class we will explore real chemical questions involving equilibrium, acid base chemistry, electrochemistry, surface phenomena and solution chemistry by reading and discussing research papers.

COURSE CONTENT:

Entropy and Information

- Absolute temperature
- Shannon Entropy

Thermodynamics & Thermochemistry

- First, second and third laws of thermodynamics and their applications in chemistry
- Enthalpy change and its impact on material science and biology
- Enthalpies of formation and reaction enthalpies
- Internal energy, entropy, Gibbs free energy
- Ideal Gas Law
- Kinetic Theory of Gases
- Design of an air bag
- Maxwell-Boltzmann Distribution

Phase Equilibria

- Phase diagrams and impact on material sciences
- Phase transitions
- Chemical equilibrium and its impact on technology and biochemistry
- Changes in equilibria with temperature and pressure
- Colligative properties
- Raoult's Law
- Ideal and non-ideal mixtures

Acid-base equilibria

- Open systems
- Soil Equilibria & Acid Rain

Chemical Kinetics

- Determination of rate, order and rate laws
- Impact of Chemical Kinetics on Biochemistry
- Oxidation of glucose in biological systems

Catalysis

- Activation energy
- Arrhenius equation
- Kinetics; Mechanisms; Enzymes
- Reducing Air Pollution from Automobiles

Diffusion across membranes

- Osmosis and reverse osmosis
- Design of a water filter
- Adsorption and Chromatography
- Ion Exchange columns and water purification

Electrochemistry in biology

- Nernst Equilibrium Potential
- Voltage-gated ion channels
- Photosynthesis and solar cells

Protein-ligand binding

- Binding free energy
- Force fields
- Empirical potentials
- Conformational freedom
- Docking & scoring computer lab

Statistical Thermodynamics

- Microcanonical, Canonical and Grand Canonical Ensembles
- Partition function
- Molecular Dynamics computer lab
- Monte Carlo simulations computer lab
- Membrane Protein Simulations computer lab

Molecular Reaction Dynamics

- Transition State
- Effect of translational and vibrational kinetic energy

Prerequisites: Chemical Principles (CHY111).

CHY212: **Chemical Applications of Group Theory** (2 credits: 2 Lectures) Monsoon

COURSE CONTENT:

Symmetry operations and symmetry elements, Concepts and properties of a group, group multiplication Tables, Similarity transformation, Class, Determination of symmetry point group of molecules, Matrix representation of groups, reducible and irreducible representations, Great orthogonality theorem, Character tables, Direct Product and Spectroscopic selection rule, Molecular Vibrations, Normal coordinates, Symmetry of normal mode vibrations, Symmetry Adapted Linear Combination, Infrared and Raman active vibrations, Molecular orbitals, LCAO MO approach, HMO method, Hybrid orbitals, Free ion configuration, terms and states, splitting of levels and terms in a chemical environment, correlation diagrams, spectral and magnetic properties of the transition metal complexes.

Course outline:

- *Introduction*: Importance of Group Theory in Chemistry
- *Symmetry elements and symmetry operations*: Use molecular models to identify symmetry elements of different molecules. Understanding of the interrelation of different symmetry elements present in a molecule, product of symmetry operations.
- *Point Groups*: Concepts and properties of a group, group multiplication Tables, Similarity transformation, Class, Determination of symmetry point group of molecules.
- *Matrix representations and Character Tables*: Matrix representation of groups, reducible and irreducible representations, Great orthogonality theorem, character tables.
- *SALC, direct product, Molecular vibrations*: Direct Product and Spectroscopic selection rule, Molecular Vibrations, Normal coordinates, Symmetry of normal mode vibrations, Symmetry Adapted Linear Combination, Infrared and Raman active vibrations.
- *Molecular orbital Theory, Hybrid orbitals*: Molecular orbitals, LCAO MO approach, HMO method, Hybrid orbitals.
- *Terms and states, Transition metals chemistry*: Free ion configuration, terms and states, splitting of levels and terms in a chemical environment, correlation diagrams, spectral and magnetic properties of the transition metal complexes.

Prerequisites: Chemical Principles (CHY111); Mathematical Methods.

CHY213: **Physical Methods in Chemistry** (4 credits: 3 Lectures + 3-hour Lab) Monsoon

Analyses of compounds are an integral aspect of chemistry. We get to know the structure, spatial orientation and purity of compounds we synthesize through analysis which helps us to advance in our investigation. To address this purpose a bevy of instruments ranging from UV spectroscopy, IR spectroscopy to High Pressure Liquid Chromatography are available. However accurately understanding the output from these instruments is an essential attribute for a successful chemist. The purpose of this course is to familiarize the students with the basic principles of spectroscopic and diffraction methods that are instrumental to the analysis of molecules and structures in the day-to-day life of a chemist. In this course, we will learn to interpret and understand working of various types of analytical instruments commonly used for analysis in a chemistry lab.

COURSE CONTENT:

UV-visible spectroscopy: Beer – Lambert law, types of electronic transitions, effect of conjugation. Concept of chromophore and auxochrome. Bathochromic, hypsochromic, hyperchromic and hypochromic shifts, Woodward – Fieser rules, Woodward rules, introduction to fluorescence.

Vibrational spectroscopy: Molecular vibrations, Hooke's law, Modes of vibration, Factors influencing vibrational frequencies: coupling of vibrational frequencies, hydrogen bonding, electronic effects, The Fourier Transform Infrared Spectrometer, Calibration of the Frequency Scale, Absorbance and Transmittance scale, intensity and position of IR bands, fingerprint region, characteristic absorptions of various functional groups and interpretation of IR spectra of simple organic molecules, basic mention of Raman Spectroscopy including the mutual exclusion principle, Raman and IR active modes of CO_2.

Nuclear Magnetic Resonance (NMR) spectroscopy: Spinning nucleus, effect of an external magnetic field, precessional motion and precessional frequency, precessional frequency and the field strength, chemical shift and its measurement, factors influencing chemical shift and anisotropic effect, proton NMR spectrum, influence of restricted rotation, solvents used in NMR, solvent shift and concentration and temperature effect and hydrogen bonding, spin-spin splitting and coupling constants, chemical and magnetic equivalence in NMR, Lanthanide shift reagents, factors influencing the coupling constant, germinal coupling, vicinal coupling, heteronuclear coupling, deuterium exchange, proton exchange reactions.

Electron Spin Resonance Spectroscopy: Derivative curves, g values, Hyperfine splitting

X-ray Diffraction: X-ray and diffraction of X-rays by atoms, Bragg's law, lattice, crystal systems, planes and Miller indices, reciprocal lattice, crystal growth and mounting, diffractometer operation, recording diffraction pattern, reflection analysis and preliminary structure determination. ,

Mass spectrometry: Basic principles, basic instrumentation, electron impact ionization, separation of ions in the analyzer, isotope abundances, molecular ions and metastable ions, basic fragmentation rules, factors influencing fragmentation, McLafferty rearrangements, chemical ionization.

Data Analysis: Uncertainties, errors, mean, standard deviation, least square fit.

Prerequisites: Chemical Principles (CHY111), Basic Organic Chemistry-I (CHY122).

CHY221: **Basic Organic Chemistry-II** (4 credits: 2 Lectures + 1 Tutorial + 3-hour Lab) Monsoon

Organic reactions; nucleophilic substitution, elimination, addition and electrophilic aromatic substitution reactions with examples will be studied.

COURSE CONTENT:

A. Substitution reactions:

Free radical halogenation, relative reactivity and selectivity, allylic and benzylic bromination

Nucleophilic Subsititution (S_N1, S_N2, S_N1', S_N2',S_Ni)

Electrophilic Substitution (S_NAr, Addition Elimination vs. Elimination addition)

Electrophilic aromatic substitution will be studied in detail

B. Elimination reactions:

Formation of alkenes and alkynes by elimination reactions, Mechanism of E1, E2, E1cB reactions. Saytzeff and Hofmann eliminations.

C. Addition reactions:

a. Alkanes sigma bonds

Chemistry of alkanes: Formation of alkanes, Organometallic reagents, Wurtz reaction, Wurtz-Fittig reactions.

b. Alkenes and alkynes pi bonds

Electrophilic additions their mechanisms (Markownikoff/ Anti-Markownikoff addition), mechanism of oxymercuration-demercuration, hydroboration oxidation, ozonolysis, reduction (catalytic and chemical), syn and anti-hydroxylation(oxidation). 1,2-and 1,4-addition reactions in conjugated dienes and Diels-Alder reaction; electrophilic and nucleophilic additions. Hydration to form carbonyl compounds, alkylation of terminal alkynes.

Prerequisites: Chemical Principles (CHY111), Basic Organic Chemistry-I (CHY122).

CHY222: **Chemistry of Carbonyl Compounds** (4 credits: 2 Lectures + 1 Tutorial + 3-hour Lab) Spring

COURSE CONTENT:

1. Nucleophilic Addition:
   (a) Reactivity of carbonyl groups
   (b) Cyanide as nucleophile- cyanohydrin formation
   (c) Oxygen/sulfur as nucleophile - Acetals, Ketals and Hydrates
   (d) Hydride as the nucleophile - Reduction reactions
   (e) Carbon as nucleophile - Organometallics (Grignard and alkyl lithiums)
   (f) Nitrogen as nucleophile - Imine and hydrazones.
   (g) Nucleophilic addition to carbonyl analogs

2. Nucleophilic Substitution:
   (a) Reactivity of carboxylic acid family
   (b) Oxygen/sulfur as nucleophile – Esters and carboxylic acids
   (c) Nitrogen as nucleophile – Amides
   (d) Acyl halides and anhydrides
   (e) Hydride as the nucleophile - Reduction reactions
   (f) Carbon as nucleophile - Organometallics (Grignard and alkyl lithium)
   (g) Enantiomer resolution
   (h) Nucleophilic Substitution at sulfuric and phosphoric acids

3. The alpha carbanion – nucleophilic-electrophilic reactivity of carbonyls
   (a) Enols and enolate anions
   (b) Addition-dehydration – The aldol reaction
   (c) Ester condensation
   (d) Fragmentation of Beta-dicarbonyl compounds
   (e) Alkylation of enolate anions
   (f) Other stabilized carbanions and carbon nucleophiles

4. Nucleophilic additions and substitutions in Synthesis
   (a) Available reactions
   (b) Experimental considerations
   (c) The strategy of synthesis
   (d) Synthesis examples

Prerequisites: Basic Organic Chemistry-I (CHY122), Basic Organic Chemistry-II (CHY221).

CHY 241: **Electrochemistry** (4 credits: 3 Lectures) Monsoon

1. Electrical dimensions and unit, Faraday's laws of electrolysis, Theory of electrolytic dissociation, van't Hoff factor and degree of dissociation, Specific Conductance, Equivalent conductance, Equivalent conductance at

infinite dilution, Variation of equivalent conductance with concentration for strong and weak electrolytes, Conductance ratio and degree of dissociation, Equivalent conductance minima, Influence of dielectric constant on conductance, Kohlrausch's law, Application of ion conductance, Ionic mobility, Influence of temperature on ionic conductance, Ion conductance and viscosity, Drift Speed, Variation of ionic mobility with ionic size and hydrodynamic radius, factors affecting the ionic mobility for strong electrolytes, Ionic Atmosphere, relaxation effect or asymmetry effect, Electrophoretic effect, partial molar quantities (briefly), partial molar free energy and chemical potential, Electrolytes as a non-ideal solution, activity coefficient, mean ionic activity, mean ionic molality, mean ionic activity coefficient, Outline of Debye-Hückel theory, Debye-Hückel's limiting law, variation of activity coefficient with ionic strength, Nernst equation.

2. General discussion about oxidation and reduction, electron transfer vs atom transfer, oxidation no.
3. Concept of electrochemistry, Definition: Electrochemical cell, electrodes, salt bridge and its function etc. Battery; types of cell: Electrolytic cell vs Galvanic cell; concentration cell vs chemical cell, construction of a voltaic cell.
4. Definition: Electrode potential, Std. potential and Formal potential; Physical significance of electrode potential.
5. Types of electrodes: (i) metal electrode, advantage of amalgam electrode; (ii) non-metal electrode, e.g. hydrogen gas electrode, glassy carbon electrode. What is glassy carbon electrode? What is the difference between glassy carbon and graphite electrode?
6. Factors affecting the electrode potential: (i) effect of concentration, (ii) effect of pH e.g. formation of insoluble hydroxide and (iii) effect of precipitation and complexation.
7. Application of electrode potential; Periodic trend of the reduction potential; Pourbaix diagram.
8. Electroanalytical techniques: Potentiometry, Coulometry, Voltammetry and Amperometry.
9. Measurement of electrode potential; 3 electrode system: working electrode, reference electrode and counter electrode; comparison between three and two electrode system; linear sweep voltammetry, Cyclic voltammetry (CV), Differential pulse voltammetry (DPV) etc.
10. Bulk electrolysis.

Prerequisite: Chemical Principles (CHY111)

Co-requisites: Chemical Equilibrium (CHY211).

CHY242: **Coordination Chemistry** (4 credits: 3 Lectures + 3-hour Lab) Spring

Metals ions play important role in producing colour in coordination complexes. Understanding of the coordination complexes lies at the heart of coordination chemistry. This course will focus on the basic concept of coordination chemistry and their quantification in photophysical and magnetic properties. Students will synthesize interesting colour compounds and perform reactions to promote the understanding of common reactions. Intensive use of analytical and spectroscopic techniques to interpret extent of reaction, purity of product and photophysical property particularly colour of the coordination complexes will be involved.

COURSE CONTENT:

Introduction and structures of complexes: Meaning of metal coordination and use of metal coordination in formation of color complex. Coordination number, bonding of organic ligands to transition metals, coordination number, linkage isomerism, electronic effects, steric effects, the chelate effect, fluxional molecules.

Crystal field theory: application and limitation; Molecular orbital theory: Application in π-bonding, electronic spectra including MLCT, LMCT d-d transition, and magnetic properties of complexes.

Inorganic substitution reaction; Types; Base catalyzed hydrolysis; Linear free energy relationship.

Reaction and kinetics: Nucleophilic substitution reactions, rate law, mechanism of reactions, trans effect, ligand field effect, inner sphere and outer sphere reactions.

Prerequisites: Chemical Principles (CHY111) and Chemical equilibrium (CHY211).

In-Depth Courses: In-depth courses provide not only advanced instruction, but also development of critical thinking and problem-solving skills and computational data analysis and modelling. Students are expected to be able to define problems clearly, develop testable hypotheses, design and execute experiments, analyse data using appropriate statistical methods, and draw appropriate conclusions, applying an understanding of all chemistry sub-disciplines. Students are also expected to be able to use the peer-reviewed scientific literature effectively and evaluate technical articles critically, learning how to retrieve specific information from the chemical literature, with the use of online, interactive database-searching tools.

CHY311: **Chemical Binding** (4 credits: 3 Lectures + 2-hour Computer Lab) Monsoon

Quantum mechanics provides the microscopic basis for a fundamental understanding of chemistry, molecular structure, bonding, and reactivity. This course and the associated computer lab provide a comprehensive treatment of valence bond and molecular orbital theories, post Hartree-Fock wave function and density functional methods. Students will learn to compute molecular structures, spectra, and thermochemical parameters for molecules in the gas-phase and for condensed-phase systems.

COURSE CONTENT:

- Postulates of Quantum Mechanics
- Atomic Orbitals and Basis Sets
- The Born-Oppenheimer approximation and the molecular Hamiltonian
- The Concept of the Potential Energy Surface
- Geometry Optimization and Frequency Analysis
- Semi-empirical and *ab initio* Quantum Mechanics
- Variation and Perturbation Theory
- Valence Bond and Molecular Orbital theories
- Independent-Particle Models: the Hartree method
- Spin, statistics and the Pauli principle
- The Hartree-Fock Self-Consistent Field equations
- Electron Correlation, Density Matrices and Natural Orbitals
- Density Functional Theory
- Periodic systems
- Implicit and explicit solvent methods
- QM/MM and ONIOM

Prerequisites: Chemical Principles, Calculus, Linear Algebra, physics, CS.
Co-requisite: Molecular Spectroscopy.

CHY313: **Molecular Spectroscopy** (3 credits: 3 Lectures) Monsoon

COURSE CONTENT:

Blackbody radiation, Einstein A and B coefficients, absorption and emission of radiation, lineshape functions, natural Lifetime broadening, pressure broadening, Doppler broadening.

Molecular symmetry, symmetry elements and symmetry operations, groups, point group, similarity transformations and classes, matrix representation of groups, reducible and irreducible representations, Great Orthogonality Theorem, character tables, Mulliken notation, matrix representation of the Schrodinger equation, Born-Oppenheimer approximation, symmetry of the Hamiltonian operator, projection operators, direct product representations, integrals and selection rules.

Rotational Spectroscopy: Rotation and rigid bodies, moment of inertia tensor and principal axis, diatomic and linear molecule: selection rule, centrifugal distortion, rotational line intensities for diatomic and linear molecule, symmetric tops.

Vibrational Spectroscopy: Diatomic molecules, wave function for harmonic and anharmonic oscillator, , selection rule, spectrum for harmonic and anharmonic oscillator, Fundamental, overtone, diatomic vibrating rotator and vibration-rotation spectrum: P, Q, R branches, vibrations of polyatomic molecules, Normal mode coordinates and their symmetry, Determining Infrared active vibrations from character table

Light scattering and the Raman effect, classical model of Raman effect, Polarizability tensor, Stokes scattering and Anti stokes scattering, Depolarization ration in Raman, Rotational Raman spectrum for diatomic and linear molecules and symmetric tops, Rule of Mutual exclusion, vibrational Raman spectrum, Raman activity of vibrations from character table.

Electronic Spectroscopy: Electronic wave function, hydrogen atom spectrum, orbital angular momentum, electron spin angular momentum, total electronic angular momentum, fine structure of hydrogen atom spectrum, many electron atoms, term symbols, Zeeman effect, electronic spectra of diatomic molecules, vibrational progressions, Frank-Condon principle, Rotational Fine structure, Fortrat diagram, electronic angular momentum for diatomic molecules, spectrum of molecular hydrogen, photoelectron spectroscopy; Fluorescence spectroscopy.

NMR: relaxation, 2-D NMR, Bloch equation, factors influencing the coupling constant, germinal coupling, vicinal coupling, heteronuclear coupling, deuterium exchange, simplification of complex spectra in NMR: spin decoupling and Lanthanide shift reagents, Nuclear Overhauser effect (NOE), resonance of other nuclei. 13C NMR: Chemical shift, 13C coupling constants, two-dimensional NMR spectroscopy, NOESY, DEPT, INEPT terminology.

Prerequisites: Physical Methods in Chemistry (CHY213); Chemical Applications of Group Theory (CHY312).

Co-requisite: Chemical Binding (CHY311).

CHY321: **Named Organic Reactions and Mechanisms** (3 credits: 3 Lectures) Monsoon

COURSE CONTENT:

C-C bond forming reactions and their mechanism focusing on Carbanion alkylation, Carbonyl addition and carbonyl substitution reactions, Conjugate addition reactions (1,2-addition & 1,4- addition), Reactions of alkene, alkynes and aromatics. C-N and C-O bond forming reactions and their mechanism. Glycosylation reactions. Oxidation and reduction reactions, Rearrangement reactions, Free radical reactions. Photochemical reactions and mechanism, Norrish type I and II reactions, Electrophilic substitution reactions. These types of reactions will be taught under following name reactions.

A. C-C Bond forming reactions and Mechanism

Grignard Reaction, Aldol Condensation, Diels Alder Reaction, Ring Closing Metathesis, Heck Reaction, Negishi Reaction, Suzuki Reaction, Benzoin condensation, Reformatsky reaction, Ugi reaction, Wittig reaction, Morita-Baylis-Hillmann Reaction.

B. C-N Bond forming reactions and Mechanism

Ullmann reaction, Buchwald and Hartwig reaction, Metal free C-N bond formation reactions, Fisher Peptide synthesis, Hetero Diels Alder reaction, Click reaction.

C. C-O Bond forming reactions and Mechanism

Allan-Robinson Reaction, Baeyer-Villiger Reaction, Fisher Oxazole synthesis, Ferrier Reaction, Glycosidation reaction, Sharpless asymmetric Epoxidation.

D. Oxidation, Reduction reactions and Mechanism

Bayer-Villeger oxidation, Dess-Martin periodinane oxidation, Swern Oxidation, Corey–Kim oxidation, Jones Oxidation, Luche reduction, Birch reduction, Gribble reduction.

E. Rearrangement Reactions and Mechanism

Benzilbenzilic acid rearrangement, Pinacol Pinacolone rearrangement, Fries rearrangement, Amadori rearrangement, Beckmann rearrangement, Demzanov rearrangement, Payne rearrangement, Wallach rearrangement, Ferrier rearrangement

F. Conjugate addition reactions and Mechanism

1,2-addition reaction, 1,4-addition reaction, Reformatsky reaction, Prins reaction, Michael reaction

G. Photochemical reactions and Mechanism

Norish type I reaction, Norish type II reaction

Prerequisites: Basic Organic Chemistry-II (CHY221).

CHY322: **Organic Reaction and Synthesis** (3 credits: 3 Lectures) Spring

COURSE CONTENT:

a. Electrophilic addition to carbons
   i. Electrophilic aromatic substitution
   ii. Common heterocycles and their reactions
   iii. Electrophilic addition to carbon-carbon multiple bonds.

b. Rearrangement reactions
   i. Migration to C, N, O and B
   ii. Free radical rearrangements
   iii. Anion rearrangement
   iv. Sigmatropic rearrangements

c. Oxidation and Reduction reactions
   i. Oxidation/Reduction of carbonyls
   ii. Reductive elimination and fragmentation
   iii. Olefin reduction
   iv. Reductive deoxygenation of carbonyl groups

v. Chemoselective oxidation and reduction reactions of functional groups

d. Cycloaddition, unimolecular rearrangement and thermal eliminations
   i. Name reactions and mechanism
   ii. Applications and limitations of the major reactions in organic synthesis
   iii. Application in natural product synthesis
   iv. Literature review

e. Reaction involving transition metals
   i. Name reactions and mechanism,
   ii. Applications and limitations of the major reactions in organic synthesis.
   iii. Application in natural product synthesis
   iv. Literature review

Each topic will end with a discussion section, where student participation is important.

Prerequisites: Basic Organic Chemistry-II (CHY221).

CHY323: **Organometallic Chemistry** (3 credits: 3 Lectures) Monsoon

The course will discuss various organometallic compounds involving Pd, Pt, Cr, Mo, Mn, their various complexes with several organic ligands and their application in the synthesis of heterocycles and natural products. The course will also cover all the name reactions involving organometallics. Since the advent of Pd as a suitable metal for C-C bond formation along with Ru-in Grubbs Metathesis the present pharmaceutical industry relies heavily on organometallics. Nearly 40% of the reactions in the lab involve organometallics. The intricacies of the reactions, the subtlety of the condition in the reactions involving organometallic compounds requires utmost understand of the mechanism of the reactions. Hence this course will provide an in-depth understanding of organometallic reactions and their applications.

COURSE CONTENT:

1. Definition: Organometallic compound, 18 electron rule, explanation from molecular orbital theory, Back bonding in terms of CO stretching frequency, structure of polynuclear carbonyl complexes. Phosphine and related ligands, Tollman cone angel; pi-bonded organic ligand; H_2, N_2 and O_2 as ligand; Metal alkyl, carbine and carbine complexes; Ferrocene and other metallocenes.
2. Basic organometallics reactions: Insertion, Oxidative addition, Reductive elimination; ß-Hydrogen elimination.
3. Homogeneous catalysis by soluble transition metal complexes: Hydroformylation; Hydrogenation; Olefin Metathesis etc.
4. C-H activation: Introduction, C-H functionalization vs. C-H activation, Importance, Classification, Organometallic C-H activation vs biological C-H activation; Present research status.
5. Synthetic Applications
   i. Synthetic Applications of Transition Metal Carbonyl Complexes
   ii. Synthetic Applications of Transition Metal Carbene Complexes
   iii. Synthetic Applications of Transition Metal Alkene, Diene, and Dienyl Complexes
   iv. Synthetic Applications of Transition Metal Alkyne Complexes
   v. C-C coupling reactions, mechanism, Present research status

Prerequisites: Basic Organic Chemistry-II (CHY221), Coordination Chemistry (CHY242).

CHY332: **Informatics & Molecular Modelling** (3 credits: 2 Lectures + 2-hr computer lab)

This course and the associated computer lab deal with Molecular Modelling and Cheminformatics, applied to the search for new drugs or materials with specific properties or specific physiological effects (*in silico* Drug Discovery). Students will learn the general principles of structure-activity relationship modelling, docking & scoring, homology modelling, statistical learning methods and advanced data analysis. They will gain familiarity with software for structure-based and ligand-based drug discovery. Some coding and scripting will be required.

COURSE CONTENT:

1. Introduction:
    - Drug Discovery in the Information-rich age
    - Introduction to Pattern recognition and Machine Learning
    - Supervised and unsupervised learning paradigms and examples
    - Applications potential of Machine learning in Cheminformatics & Bioinformatics
    - Introduction to Classification and Regression methods

2. Representation of Chemical Structure and Similarity:

    - Sequence Descriptors
    - Text mining
    - Representations of 2D Molecular Structures: SMILES
    - Chemical File Formats, 3D Structure
    - Descriptors and Molecular Fingerprints
    - Graph Theory and Topological Indices
    - Progressive incorporation of chemically relevant information into molecular graphs
    - Substructural Descriptors
    - Physicochemical Descriptors
    - Descriptors from Biological Assays
    - Representation and characterization of 3D Molecular Structures
    - Pharmacophores
    - Molecular Interaction Field Based Models
    - Local Molecular Surface Property Descriptors
    - Quantum Chemical Descriptors
    - Shape Descriptors
    - Protein Shape Comparisons, Motif Models
    - Molecular Similarity Measures
    - Chemical Space and Network graphs
    - Semantic technologies and Linked Data

3. Mapping Structure to Response: Predictive Modelling:
    - Linear Free Energy Relationships
    - Quantitative Structure-Activity/Property Relationships (QSAR/QSPR) Modeling
    - Ligand-Based and Structure-Based Virtual High Throughput Screening
    - 3D Methods - Pharmacophore Modeling and alignment
    - ADMET Models
    - Activity Cliffs
    - Structure Based Methods, docking and scoring
    - Model Domain of Applicability

4. Data Mining and Statistical Methods:
    - Linear and Non-Linear Models

- Data preprocessing and performance measures in Classification & Regression
- Feature selection
- Principal Component analysis
- Partial Least-Squares Regression
- kNN, Classification trees and Random forests
- Cluster and Diversity analysis
- Introduction to kernel methods
- Support vector machines classification and regression
- Introduction to Neural Nets
- Self-Organized Maps
- Deep Neural Networks
- Introduction to evolutionary computing
- Genetic Algorithms
- Data Fusion
- Model Validation
- Best Practices in Predictive Cheminformatics

Prerequisites: Basic Organic chemistry/Biochemistry, Basic Statistics, Computer Programming.

CHY342: **Chemistry of Solids and Surfaces** (3 credits: 3 Lectures) Spring

In this course the students will get to know the chemistry behind the formation of solids and on their surfaces, the kind of bonding involved and the available techniques to characterize them. Through this course students will also learn how to interpret various chemical structures of solids and their surfaces. Students will further understand crystallographic terminology, selected diffraction theory, nomenclature at surfaces, reconstruction and relaxations at surfaces and how to determine the surface structure. They will also realize the wide range of chemical information available from diffraction based techniques. Further the students will learn about different surface phenomena such as adsorption, catalysis, work function, and basics of the electronic, magnetic, and optical properties, and their relevance to nanomaterials. This is a required course for Chemistry majors, but also satisfies UWE requirements for non-majors.

COURSE CONTENT:

- INTRODUCTION TO SOLID STATE CHEMISTRY
- CRYSTAL CHEMISTRY
  - Introduction to Crystallography
  - Unit cells and Crystal Systems
  - Symmetry, Lattice, Lattice spacing
  - Crystal Densities and Packing
  - Crystallographic Notations
- BONDING IN SOLIDS
  - Overview on Bonding
    - Ionic, Covalent, Metallic, van der Waals and Hydrogen Bonding
  - Born-Haber Cycle
  - The Shapes of Molecules
  - Intermolecular Forces
- CRYSTALLINE MATERIALS
  - Properties of X-Rays

- X-Ray Emission & Absorption
- X-Ray Diffraction Techniques
- Point, Line, Interface & Bulk Defects

- AMORPHOUS MATERIALS
  - Introduction to Glasses
  - Glass Properties

- INTRODUCTION TO THE CHEMISTRY of SURFACES

- Surface structure

  Nomenclature

  Surface unit cell

  Relaxation and reconstruction at surfaces and its relevance to nanomaterials

  How to characterize atomic structure at surfaces

- Basics of different phenomena at surfaces

  Surface energy

  Electronic structure, 2D Brillouin zone, photoemission

  Work function

  Magnetic properties and relevance to nanomaterials

  Optical properties

  Adsorption and catalysis

  Two dimensional structures

Prerequisites: Chemical Principles (CHY111), Physics (PHY101/102 or PHY103/104).

CHY344: **Topics in Nanotechnology** (3 credits: 3 Lectures) Spring

The next few years will see dramatic advances in atomic-scale technology. Molecular machines, nanocircuits, and the like will transform all aspects of modern life - medicine, energy, computing, electronics and defense are all areas that will be radically reshaped by nanotechnology. These technologies all involve the manipulation of structures at the atomic level - what used to be the stuff of fantasy is now reality. The economics impact of these developments has been estimated to be in the trillions of dollars. But, as with all new technologies, ethical and legal challenges will arise in their implementation and further development. This course will examine the science of nanotechnology and place it in the larger social context of how this technology may be, and already is, applied. Underlying physical science principles will be covered in lecture sessions and students will read articles from current news sources and the scientific literature. There will be presentations on scientific literature on topics of student interests, to examine the science and applications of a well-defined aspect of nanotechnology of their choosing. Lecture material will focus on the principles behind modern materials such as semi-conductors (organic, inorganic) and novel nanostructures.

COURSE CONTENT:

- Introduction
- Bulk Vs. Nano
- Quantum confinement effect
- Surface area to volume ratio

- Effect on Properties: Material (electrical, magnetic, mechanical etc.) and structural properties
- Carbon nano-architectures: Fullerene, SWNT, MWNT, Graphite etc., Classification of structure
- Q-Dots
- Bonding parameters
- Methods of preparation
- Nanomaterial's synthesis: Top down and Bottom up approach, Physical and chemical methods Applications (Nano-machines, solar cells, coatings, MEMS, nano-medicine, sensors, miscellaneous)
- Characterization Techniques and Instruments: Microscopy SEM, TEM, AFM, X-Ray diffraction, UV-vis, Photoluminescence, Raman, FTIR, ESR, XPS, BET, DLS, Zeta potential

Prerequisites: Chemical Principles (CHY111).

CHY346: **Bio- inorganic chemistry & Chemistry of F-block elements** (3 credits: 3 Lectures) Spring

COURSE CONTENT:

1. General discussion about bioinorganic chemistry

2. Biological important elements, Biological ligands

3. Alkali and alkaline earth metal in biology: Role of Na, K (Na-K pump, chelate chemistry, SHAB theory); Mg (ATP hydrolysis and chlorophyll) and Ca

3. Importance of Oxygen, Great oxygenation event

4. Iron based chemistry in nature; Iron metabolism: Iron transport, Iron storage; Iron cycle.

5. Oxygen utilization: (i) Oxygen transport and storage (ii) Oxidases enzyme: Cytochrome c oxidase, Electron transport chain, Cytochrome c oxidase vs. Cytochrome in respiratory cycle; electron transfer reaction in biology (iii) Oxygenase: Cyt P450: Reaction mechanism (iv) Peroxidase: HRP.

6. Fe-S protein, Hydrogenase enzyme.

7. Toxicity: Superoxide dismutase and Catalase

8. Mo- containing enzyme: Nitrogenase, nitrogen cycle.

9. Co, V containing enzymes.

10. Zn containing enzymes.

11. Photosynthesis: O-H bond activation, role of Mn in OEC

12. f-orbitals and oxidation states; atoms and ion sizes (lanthanoid contractions); coordination no.

13. Spectroscopic and magnetic properties of lanthanoids and actinoids.

14. Lanthanoids metals: Complexes of Ln(III), Organometallic complexes.

15. Actinoids metals: Inorganic and Organometallic complexes of Th and U.

16. Nuclear Property: Mass defect and binding energy; Nuclear emissions (alpha and beta particles, gamma radiations); Nuclear transformations, the kinetics of radioactivity decay, units of radioactivity, Nuclear fission vs. fusion.

17. Applications of isotopes: Kinetic isotope effects, Radiocarbon dating.

Prerequisites: Coordination Chemistry (CHY242).

CHY351: **Macromolecules** (3 credits: 3 Lectures) Monsoon

In this course we will learn about cellular macromolecules namely nucleic acids, proteins, carbohydrates and lipids. The chemistry and biochemistry associated with these macromolecules will be discussed. The goal is to learn about important natural molecules, not only from a structural but from a chemical point of view as well. We will talk about the chemistry associated with these molecules, their importance and how we can interfere with it. Classes will be through a combination of group discussions, reading assignments, projects, presentations and lectures. Students are expected to do library research, write papers, and present discussion in class. Review articles and papers used in this course will be provided.

COURSE CONTENT:

1. Introduction
2. Nucleic Acid (DNA and RNA)
    - a. Background
    - b. Function and importance
    - c. Structure
    - d. Biosynthesis/replication
    - e. Chemical synthesis
    - f. Sequencing
        - i. Maxam Gilbert
        - ii. Sanger dideoxy
        - iii. Bisulfite sequencing
        - iv. Mass spectrometry
        - v. NGS
    - g. DNA chemistry
        - i. DNA damage
            1. Spontaneous depurination
            2. deamination
        - ii. Alkylation
        - iii. Oxidative DNA damage
        - iv. DNA-DNA crosslinks
        - v. DNA-Protein crosslinks
        - vi. DNA methylation and demethylation
    - h. Mutagenesis
    - i. Repair
    - j. Epigenetics
    - k. RNA editing
    - l. Ribozymes
    - m. Diseases and carcinogenesis
3. Proteins
    - a. What are proteins
    - b. Functions
    - c. Amino acids

    d. Structure (primary, secondary, tertiary, quaternary)
    e. Sequencing
        i. Chemical and proteomics
    f. Peptide synthesis
    g. Enzymatic reactions
    h. Diseases
4. Lipids
    a. Functions and importance
    b. Fatty acids
    c. Phospholipids
    d. Steroids
    e. Diseases
5. Carbohydrates
    a. Introduction
    b. Function and importance in chemistry and biology
    c. Glycoconjugates
    d. Structural features
    e. Biosynthesis
    f. Chemical synthesis
    g. Industrial preparation

Prerequisites: CHY221, CHY112, Biochemistry.

CHY352: **Advanced Biochemistry** (3 credits: 2 Lectures + 3-hour Lab) Spring [REAL]

Students in this course will apply principles from general and organic chemistry, as well as general biology, to understand the molecular processes that characterize life. The goal of this class will be to give students a solid background with which they can appreciate the chemistry of life. Beginning with fundamental principles, the course will then delve into a detailed look at metabolism - the specific means by which organisms use chemical energy to drive cell functions and how they convert simple molecules to complex biological molecules. Students will have the opportunity for independent work, and will apply the principles of biochemistry to a research project that they will design, execute, and present.

Prerequisites: Chemical Principles (CHY111), Basic Organic Chemistry-I (CHY122), Essentials of Biology.

CHY 354: **Biochemical Toxicology** (3 credits: 3 Lectures) Spring

COURSE CONTENT:

1. General Principals of toxicology
2. Classes of toxicants
3. Metabolism
4. P450 and P450 catalyzed reactions
5. Other phase 1 reactions
6. Phase II/Conjugation reactions
7. Bioactivation and Reactive intermediates
8. Reaction of Chemicals with DNA
9. DNA adducts and its consequences (Mutagenesis, DNA repair and Translesion DNA synthesis)
10. Protein adducts
11. Genetic toxicology (polymorphism)

12. Molecular basis of toxicology
13. Biomarkers
14. Natural Products
15. Cellular Oncogenesis
16. Metals
17. Drug induced liver damage
18. Mass spectrometry and other analytical methods

Prerequisites: CHY111 or Basic Biochemistry.

CHY 356: **Polymers** (3 credits: 3 Lectures) Spring

The chemistry of polymers, their synthesis and characterization will form the subject matter of this advanced course, which will follow a case-study approach. Students will be expected to apply their knowledge to a real-world problem of their choice.

Prerequisites: Chemical Principles, Nature of Materials, Macromolecules.

CHY412: **Dynamics of Chemical Reactions** (4 credits)

The principles of chemical kinetics, as well as equilibrium and non-equilibrium statistical mechanics will be covered in this advanced course. The associated computer lab will introduce the student to classical and *ab initio* quantum molecular dynamics and Monte Carlo simulations of liquids and proteins. The techniques learned in this course will applied to substantive research projects that the students will design, execute, and present. Students will be encouraged to seek avenues for publication of their most significant results

Prerequisites: Chemical Equilibrium, Chemical Binding, Macromolecules.

CHY413: **Applications of analytical techniques** (3 credits: 3 Lectures) Monsoon

Applications of UV, IR, NMR, and mass spectral methods in structure elucidation /determination of organic compounds.

Pre-requisites: CHY321.

CHY417: **Theoretical Chemistry Seminar** (3 credits) [REAL]

This advanced course will cover special topics in quantum chemistry and statistical mechanics. Chemical concepts such as atoms, molecular structure, electron density, equilibrium, reaction path, etc. will also be discussed from a historical and philosophical context. Students will examine in-depth selected articles from the current scientific literature, and develop a viable research proposal in the chosen area.

Prerequisites: Chemical Binding.

CHY421: **Organic Synthesis** (4 credits) Spring [REAL]

Students will gain expertise in the techniques of organic synthesis. A major project will be the development of a research proposal based on the student's own question. Background from the literature will motivate the proposal and initial experiments will be proposed.

Prerequisites: Chemical Principles, Basic Organic Chemistry.

CHY452: **Introduction to Bio-organic Chemistry**

Basic structure of nucleic acids, proteins, lipids and carbohydrates; biological functions and biosynthesis of precursors.

CHY453: **Forensic Chemistry**

Chemistry for Forensic Scientists, Skills for Forensic Scientists Crime Scene Science, Aspects of Forensic Science, Application of Forensic Science Forensic Science Dissertation, Advances in Forensic Chemistry, Forensic Toxicology.

B.Sc. (Research) Chemistry

Recommended Semester-wise Plan

A sample path through the B.Sc. (Research) in Chemistry program is shown below, affording students flexibility in their choice of timing CCC, UWE and Chemistry Elective courses, so as to enable students to select courses of interest and to accommodate obtaining a Minor from another department.

SEMESTER 1	
Chemical Principles	5.0
Fundamentals of Physics-I	5.0
Mathematical Methods I	4.0
Computing/Programming	3.0
CCC	3.0

SEMESTER 2	
Basic Organic Chemistry I	4.0
Main Group Chemistry	3.0
Fundamentals of Physics-II	5.0
Mathematical Methods II	4.0
CCC	3.0

SEMESTER 3	
Chemical Equilibrium	5.0
Chemical Applications of Group Theory	2.0
Physical Methods in Chemistry	4.0
Basic Organic Chemistry II	4.0
Cell biology and Genetics	3.0
CCC/UWE	3.0

SEMESTER 4	
Chemistry of Carbonyl Compounds	4.0
Electrochemistry	3.0
Coordination Chemistry	4.0
Advanced Biochemistry	3.0
Probability & Statistics	4.0
CCC/UWE	3.0

SEMESTER 5	
Chemical Binding	4.0
Molecular Spectroscopy	3.0
Named Organic Reactions and Mechanism	3.0
Organometallic Chemistry	3.0
CCC	3.0
UWE	3.0

SEMESTER 6	
Organic Reaction and Synthesis	3.0
Informatics & Molecular Modelling	3.0
Chemistry of Solids and Surfaces	3.0
Bio-inorganic chemistry	3.0
CCC	3.0
UWE	6.0

SEMESTER 7	
Applications of analytical techniques	3.0
Major Electives	3.0
Senior Project	6.0
CCC/UWE	9.0

SEMESTER 8	
Major Electives	3.0
Chemistry Colloquium	1.0
Senior Project	6.0
CCC/UWE	6.0